MÖSSBAUER SPECTROSCOPY OF IRON-BASED SUPERCONDUCTOR FeSe

A. Błachowski[1], K. Ruebenbauer[1], J. Żukrowski[2], J. Przewoźnik[2], K. Wojciechowski[2], Z. M. Stadnik[4], U. D. Wdowik[1]

[1]Pedagogical University, Kraków, Poland; [2]AGH University of Science and Technology, Kraków, Poland; [3]University of Ottawa, Ottawa, Canada

Superconducting FeSe has been investigated by Mössbauer spectroscopy at various temperatures including strong external magnetic fields applied to the absorber. It was found that isomer shift exhibits sharply defined increase at about 105 K leading to the lowering of the electron density on iron nucleus by $0.02\,\mathrm{electron\ a.u.}^{-3}$. Above jump in the electron density is correlated with the transition from the *P4/nmm* to the *Cmma* structure, while decreasing temperature. Mössbauer measurements in the external magnetic field and for temperatures below transition to the superconducting state revealed null magnetic moment on iron atoms. The principal component of the electric field gradient on the iron nucleus was found as negative on the iron site. Superconductivity with the transition temperature T_c=8 K occurs for a compound being formed close to the FeSe stoichiometry. This compound has *P4/nmm* tetragonal structure at room temperature and transforms into *Cmma* orthorhombic phase between 100-80 K. It was found that T_c strongly depends upon applied pressure raising to 36.7 K at 8.9 GPa and subsequently dropping due to the induced phase transition into some hexagonal structure. Therefore, it is important to look upon phonon and electron density of states versus pressure in this unconventional compound to decide what kind of the boson field is responsible for the Cooper pairs formation. Calculations are performed for the stoichiometric compound within the density functional theory (DFT). Local density approximation (LDA) is used as better suited for the refinement of the crystal structure. A harmonic approximation is used to study lattice dynamics of the system. Results of the calculations are to be discussed in detail. Calculations show that the iron magnetic moment is zero in the ground state of both phases.

Presenting author: **Krzysztof Ruebenbauer**

Address: **PL-30-084 Kraków, ul. Podchorążych 2, Poland**

FAX: **+(48-12) 637-2243**

E-mail: **sfrueben@cyf-kr.edu.pl**